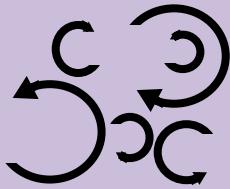
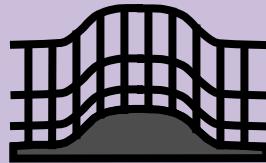


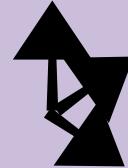
HOTMAC Mesoscale Meteorological Model



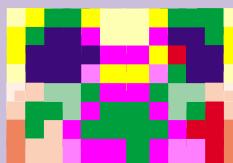
$\kappa-\epsilon$ type turbulence closure model



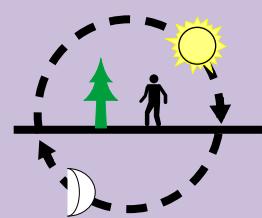
expanding vertical grid & terrain following coordinates



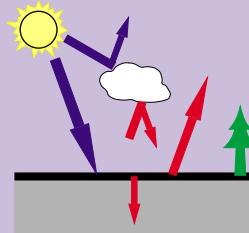
three dimensional



Thirteen surface types



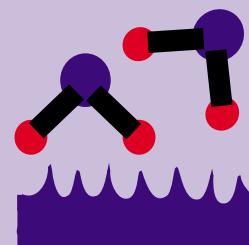
time dependent



short & long wave radiation balance (5 levels in ground)

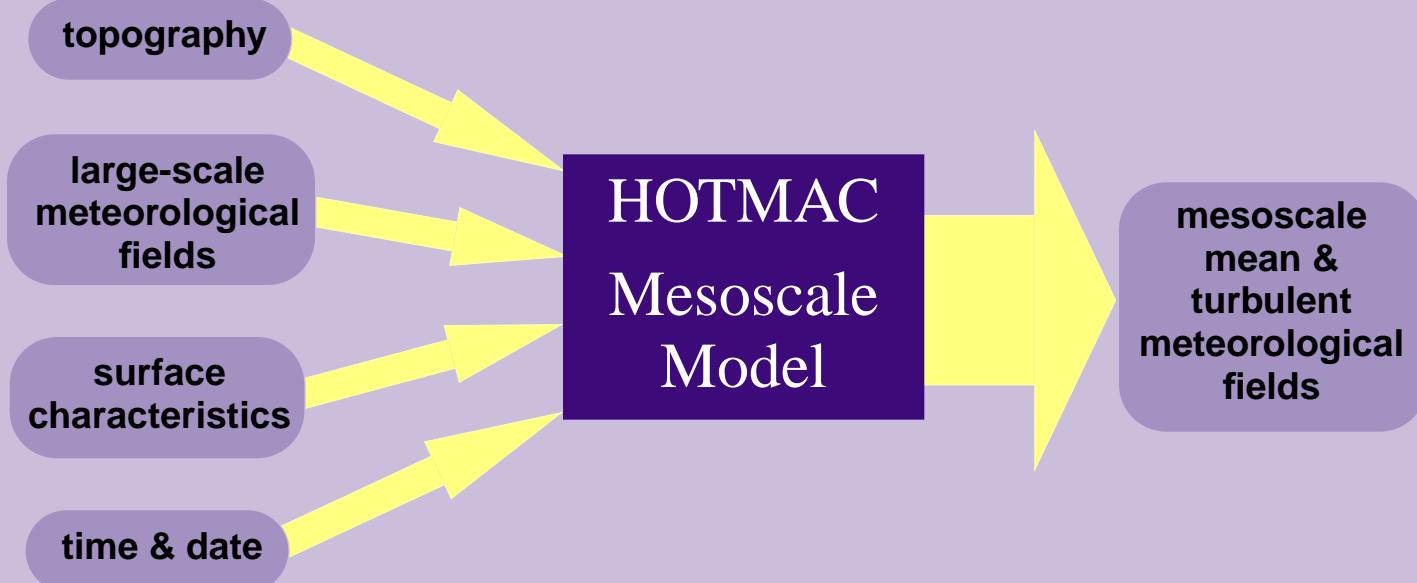


hydrostatic

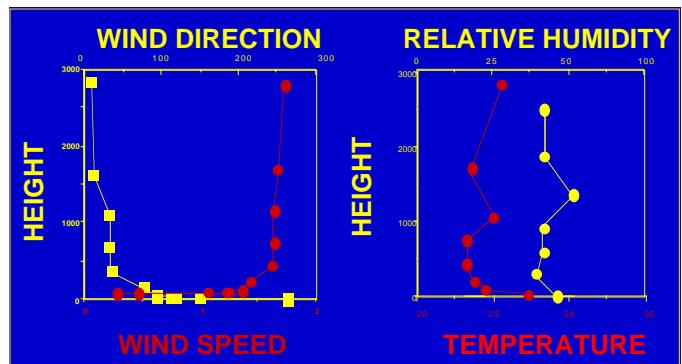


moisture, evaporation, & condensation

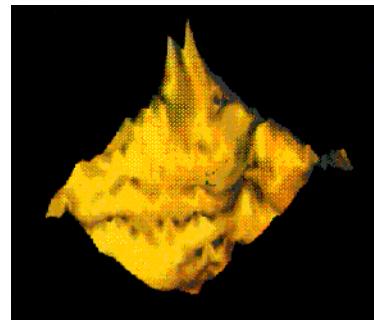
Input & Output for the HOTMAC Model



HOTMAC INPUT PARAMETERS

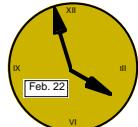


METEOROLOGICAL PROFILES



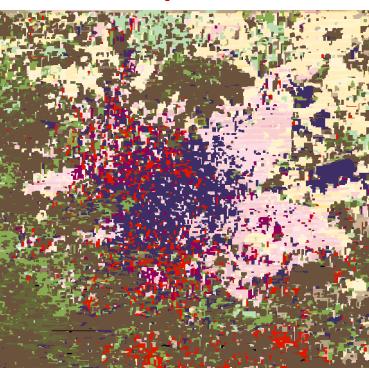
TOPOGRAPHY

TIME OF DAY



DAY OF YEAR

HOTMAC
METEOROLOGICAL
MODEL



WINDS
TURBULENCE
TEMPERATURE
MOISTURE

Governing Geophysical Flow Equations

Conservation of Mass

$$\frac{\partial \rho}{\partial t} + U_i \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial U_i}{\partial x_i} = 0$$

advection divergence/convergence

Conservation of Momentum

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + g \delta_{i3} - 2 \varepsilon_{ijk} \Omega_j U_k + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j}$$

advection pressure force gravity force Coriolis force molecular diffusion

Conservation of Heat

$$\frac{\partial \Theta}{\partial t} + U_j \frac{\partial \Theta}{\partial x_j} = -\frac{1}{\rho C_p} \frac{\partial R_j}{\partial x_j} - \frac{L_p E}{\rho C_p} + \kappa \frac{\partial^2 \Theta}{\partial x_j \partial x_j}$$

advection radiation divergence phase change molecular diffusion

Conservation of Moisture

$$\frac{\partial Q_w}{\partial t} + U_j \frac{\partial Q_w}{\partial x_j} = \nu \frac{\partial^2 Q_w}{\partial x_j \partial x_j} + S_Q$$

advection molecular diffusion source & sink terms

Reynolds Decomposition of Instantaneous Variables

$$U(t) = \bar{U} + u'(t)$$



Reynolds-averaged Advection Terms

$$U_j \frac{\partial U_i}{\partial x_j} = \bar{U}_j \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial}{\partial x_j} \bar{u'_i u'_j}$$

$$U_j \frac{\partial \Theta}{\partial x_j} = \bar{U}_j \frac{\partial \bar{\Theta}}{\partial x_j} + \frac{\partial}{\partial x_j} \bar{\theta' u'_j}$$

$$U_j \frac{\partial Q_w}{\partial x_j} = \bar{U}_j \frac{\partial \bar{Q}_w}{\partial x_j} + \frac{\partial}{\partial x_j} \bar{q' u'_j}$$

Reynolds-averaged Atmospheric Flow Equations

Continuity Equation

$$\frac{\partial \bar{U}_i}{\partial x_i} = 0$$

divergence

Conservation of Momentum

$$\frac{\partial \bar{U}_i}{\partial t} + \bar{U}_j \frac{\partial \bar{U}_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial \bar{P}}{\partial x_i} - g \frac{\delta \bar{T}}{T_0} \delta_{i3} - 2\varepsilon_{ijk} \Omega_j \bar{U}_k - \frac{\partial}{\partial x_j} \bar{u}'_i \bar{u}'_j + \nu \frac{\partial^2 \bar{U}_i}{\partial x_j \partial x_j}$$

advection	pressure force	gravity force	Coriolis force	turbulent diffusion	molecular diffusion
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Conservation of Heat

$$\frac{\partial \bar{\Theta}}{\partial t} + \bar{U}_j \frac{\partial \bar{\Theta}}{\partial x_j} = -\frac{1}{\rho_0 C_p} \frac{\partial \bar{R}_j}{\partial x_j} - \frac{L_p \bar{E}}{\rho_0 C_p} - \frac{\partial}{\partial x_j} \bar{\theta}' u'_j + \kappa \frac{\partial^2 \bar{\Theta}}{\partial x_j \partial x_j}$$

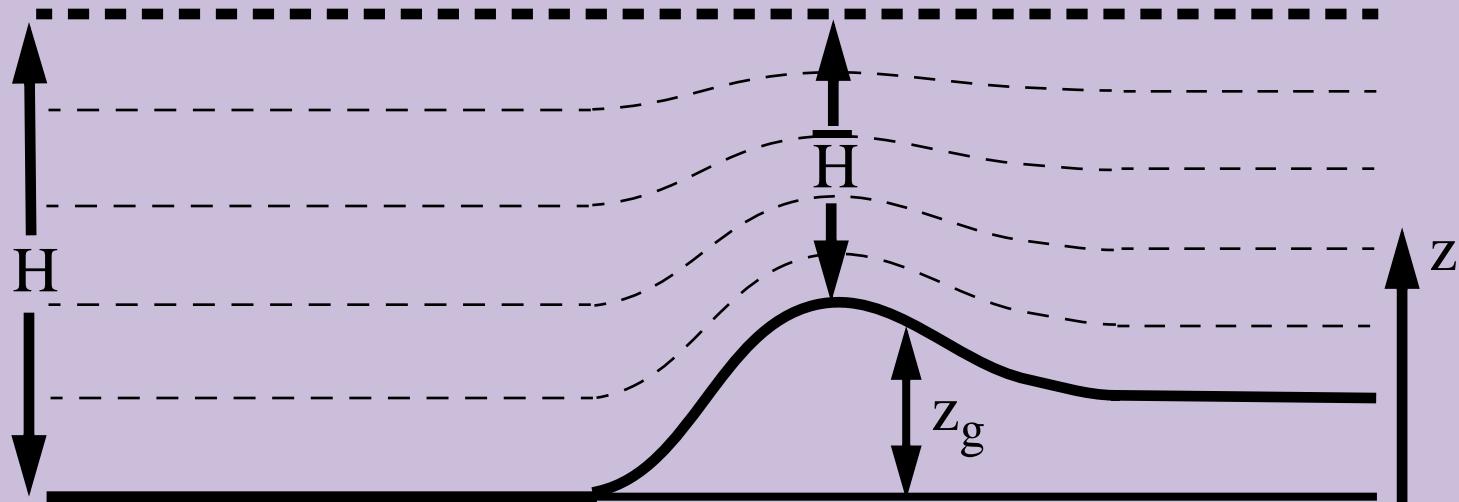
advection	radiation divergence	phase change	turbulent diffusion	molecular diffusion
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Conservation of Moisture

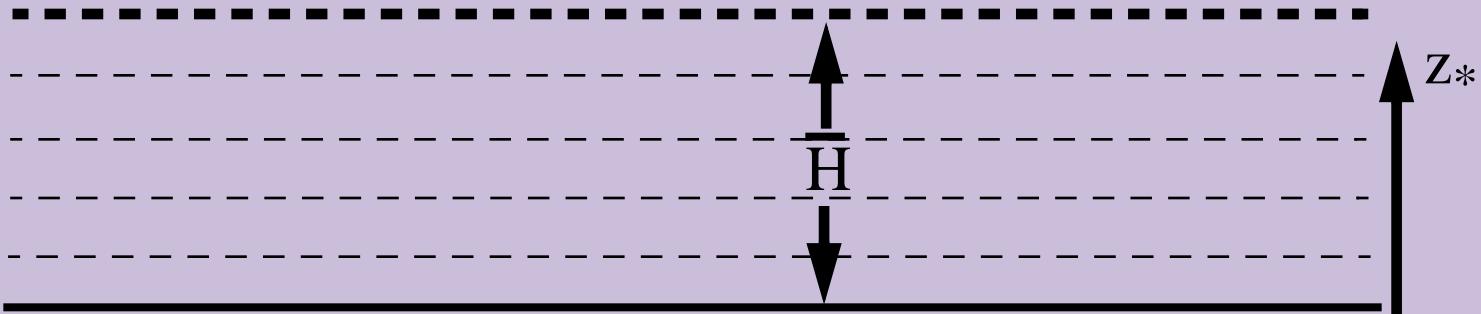
$$\frac{\partial \bar{Q}_w}{\partial t} + \bar{U}_j \frac{\partial \bar{Q}_w}{\partial x_j} = -\frac{\partial}{\partial x_j} \bar{q}' u'_j + \nu \frac{\partial^2 \bar{Q}_w}{\partial x_j \partial x_j} - \bar{S}_Q$$

advection	turbulent diffusion	molecular diffusion	source & sink terms
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Terrain-following coordinate transformation



$$z^* = \bar{H} \frac{z - z_g}{\bar{H} - z_g}$$



HOTMAC governing equations (terrain-following coords.)

Continuity Equation

$$\frac{\partial \bar{U}}{\partial x} + \frac{\partial \bar{V}}{\partial y} + \frac{\partial \bar{W}^*}{\partial z^*} - \frac{1}{H - z_g} \left(\bar{U} \frac{\partial z_g}{\partial x} + \bar{V} \frac{\partial z_g}{\partial y} \right) = 0$$

Transformation

$$z^* = \bar{H} \frac{z - z_g}{H - z_g}$$

Momentum Equations

$$\begin{aligned} \frac{D\bar{U}}{Dt} &= f(\bar{V} - \bar{V}_g) + g \frac{\bar{H} - z^*}{\bar{H}} \left(1 - \frac{\langle \bar{\Theta}_v \rangle}{\bar{\Theta}_v} \right) \frac{\partial z_g}{\partial x} + \frac{\partial}{\partial x} \left(K_x \frac{\partial \bar{U}}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{xy} \frac{\partial \bar{U}}{\partial y} \right) \\ &\quad + \frac{\bar{H}}{H - z_g} \frac{\partial}{\partial z^*} (-\bar{u}' \bar{w}') \end{aligned}$$

$$\begin{aligned} \frac{D\bar{V}}{Dt} &= -f(\bar{U} - \bar{U}_g) + g \frac{\bar{H} - z^*}{\bar{H}} \left(1 - \frac{\langle \bar{\Theta}_v \rangle}{\bar{\Theta}_v} \right) \frac{\partial z_g}{\partial y} + \frac{\partial}{\partial x} \left(K_{xy} \frac{\partial \bar{V}}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial \bar{V}}{\partial y} \right) \\ &\quad + \frac{\bar{H}}{H - z_g} \frac{\partial}{\partial z^*} (-\bar{v}' \bar{w}') \end{aligned}$$

where $\bar{W}^* = \frac{\bar{H}}{H - z_g} \bar{W} + \frac{z^* - \bar{H}}{H - z_g} \left(\bar{U} \frac{\partial z_g}{\partial x} + \bar{V} \frac{\partial z_g}{\partial y} \right)$

HOTMAC governing equations (terrain-following coords.)

Conservation of Heat

$$\frac{D\bar{\Theta}}{Dt} = \frac{\partial}{\partial x} \left[K_x \frac{\partial \bar{\Theta}}{\partial x} \right] + \frac{\partial}{\partial y} \left[K_y \frac{\partial \bar{\Theta}}{\partial y} \right] + \frac{\bar{H}}{H - z_g} \left[\frac{\partial}{\partial z^*} (-\bar{w}'\bar{\theta}') + \frac{1}{\rho C_p} \frac{\partial R_N}{\partial z^*} \right]$$

Conservation of Moisture

$$\frac{D\bar{Q}_v}{Dt} = \frac{\partial}{\partial x} \left[K_x \frac{\partial \bar{Q}_v}{\partial x} \right] + \frac{\partial}{\partial y} \left[K_y \frac{\partial \bar{Q}_v}{\partial y} \right] + \frac{\bar{H}}{H - z_g} \frac{\partial}{\partial z^*} (-\bar{w}'\bar{q}'_v)$$

Hydrostatic Assumption

Momentum Equation - vertical component

$$\frac{\partial \bar{W}}{\partial t} + \bar{U} \frac{\partial \bar{W}}{\partial x} + \bar{V} \frac{\partial \bar{W}}{\partial y} + \bar{W} \frac{\partial \bar{W}}{\partial z} = -\frac{1}{\rho_0} \frac{\partial \bar{P}}{\partial z} - g - 2\Omega_y \bar{U} - \frac{\partial}{\partial x} \bar{w'u'} - \frac{\partial}{\partial y} \bar{w'v'} - \frac{\partial}{\partial z} \bar{w'w'}$$

with hydrostatic approximation, simplifies to:

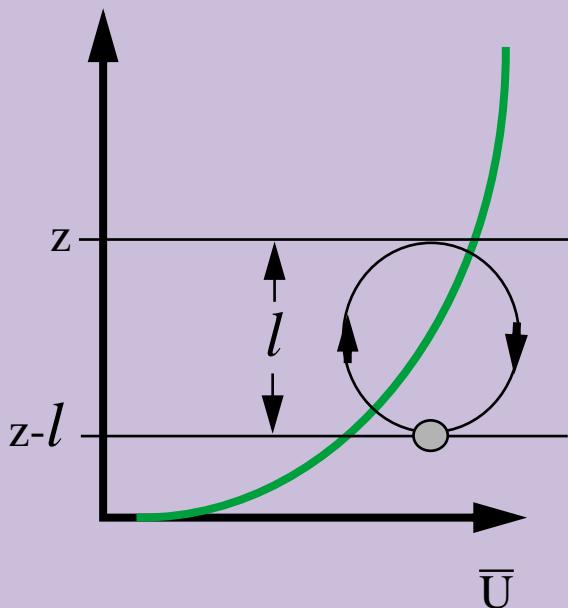
$$\frac{\partial \bar{P}_0}{\partial z} = -\rho_0 g$$

and vertical velocity obtained through the continuity eqn.:

$$-\frac{\partial}{\partial z} \bar{W} = \frac{\partial}{\partial x} \bar{U} + \frac{\partial}{\partial y} \bar{V}$$

Prandtl's Mixing Length Hypothesis

turbulent eddies transport fluid properties over finite distances resulting in turbulent fluctuations



$$u'(z) = \bar{U}(z-l) - \bar{U}(z)$$

Taylor Series Expansion:

$$u'(z) = \bar{U}(z) - 1 \frac{\partial \bar{U}(z)}{\partial z} + \frac{1^2}{2!} \frac{\partial^2 \bar{U}(z)}{\partial z^2} - \dots - \bar{U}(z)$$

$$u'(z) \approx -1 \frac{\partial \bar{U}(z)}{\partial z}$$

$$\overline{u'w'} \approx -\overline{w'} \frac{\partial \bar{U}(z)}{\partial z} = -K_{zz} \frac{\partial \bar{U}(z)}{\partial z}$$

U-eqn turbulent transport terms

$$\frac{D\bar{U}}{Dt} = \dots - \frac{\partial}{\partial x} \bar{u' u'} - \frac{\partial}{\partial y} \bar{u' v'} - \frac{\partial}{\partial z} \bar{u' w'} + \dots$$

$$\bar{u' w'} \approx - \bar{l_x w'} \cdot \frac{\partial \bar{U}}{\partial x} - \bar{l_y w'} \cdot \frac{\partial \bar{U}}{\partial y} - \bar{l_z w'} \cdot \frac{\partial \bar{U}}{\partial z} = -K_{zx} \frac{\partial \bar{U}}{\partial x} - K_{zy} \frac{\partial \bar{U}}{\partial y} - K_{zz} \frac{\partial \bar{U}}{\partial z}$$

$$\bar{u' v'} \approx - \bar{l_x v'} \cdot \frac{\partial \bar{U}}{\partial x} - \bar{l_y v'} \cdot \frac{\partial \bar{U}}{\partial y} - \bar{l_z v'} \cdot \frac{\partial \bar{U}}{\partial z} = -K_{yx} \frac{\partial \bar{U}}{\partial x} - K_{yy} \frac{\partial \bar{U}}{\partial y} - K_{yz} \frac{\partial \bar{U}}{\partial z}$$

$$\bar{u' u'} \approx - \bar{l_x u'} \cdot \frac{\partial \bar{U}}{\partial x} - \bar{l_y u'} \cdot \frac{\partial \bar{U}}{\partial y} - \bar{l_z u'} \cdot \frac{\partial \bar{U}}{\partial z} = -K_{xx} \frac{\partial \bar{U}}{\partial x} - K_{xy} \frac{\partial \bar{U}}{\partial y} - K_{xz} \frac{\partial \bar{U}}{\partial z}$$

K-theory Turbulent Closures

$$\overline{u'w'} \approx -K_{zz} \frac{\partial \bar{U}}{\partial z}$$

1st order closure

- empirical or dimensionally-derived formulae

$$K_{zz} = k u_* \Phi_m^{-1} \left(\frac{z}{L} \right)$$

$$K_{zz} = K_{\max} z \left(1 - \frac{z}{h} \right)$$

1^{1/2} order closure

- eddy diffusivity is function of **length** scale and **velocity** scale

1 eqn. model

- solve approximated equation for TKE
- prescribe equation for length scale

2 eqn. model

- solve approximated equation for TKE
- solve approximated equation for ϵ , l , or $q^2 l$

$1^{1/2}$ order two-equation model (terrain-following coords.)

$$(\bar{u}'\bar{w}', \bar{v}'\bar{w}') = -lq\tilde{S}_M \left[\frac{\partial \bar{U}}{\partial z}, \frac{\partial \bar{V}}{\partial z} \right]$$

$$(\bar{w}'\bar{\theta}', \bar{w}'\bar{q}'_v) = -\alpha lq\tilde{S}_M \left[\frac{\partial \bar{\Theta}}{\partial z}, \frac{\partial \bar{Q}_v}{\partial z} \right]$$

horizontal turbulent diffusion

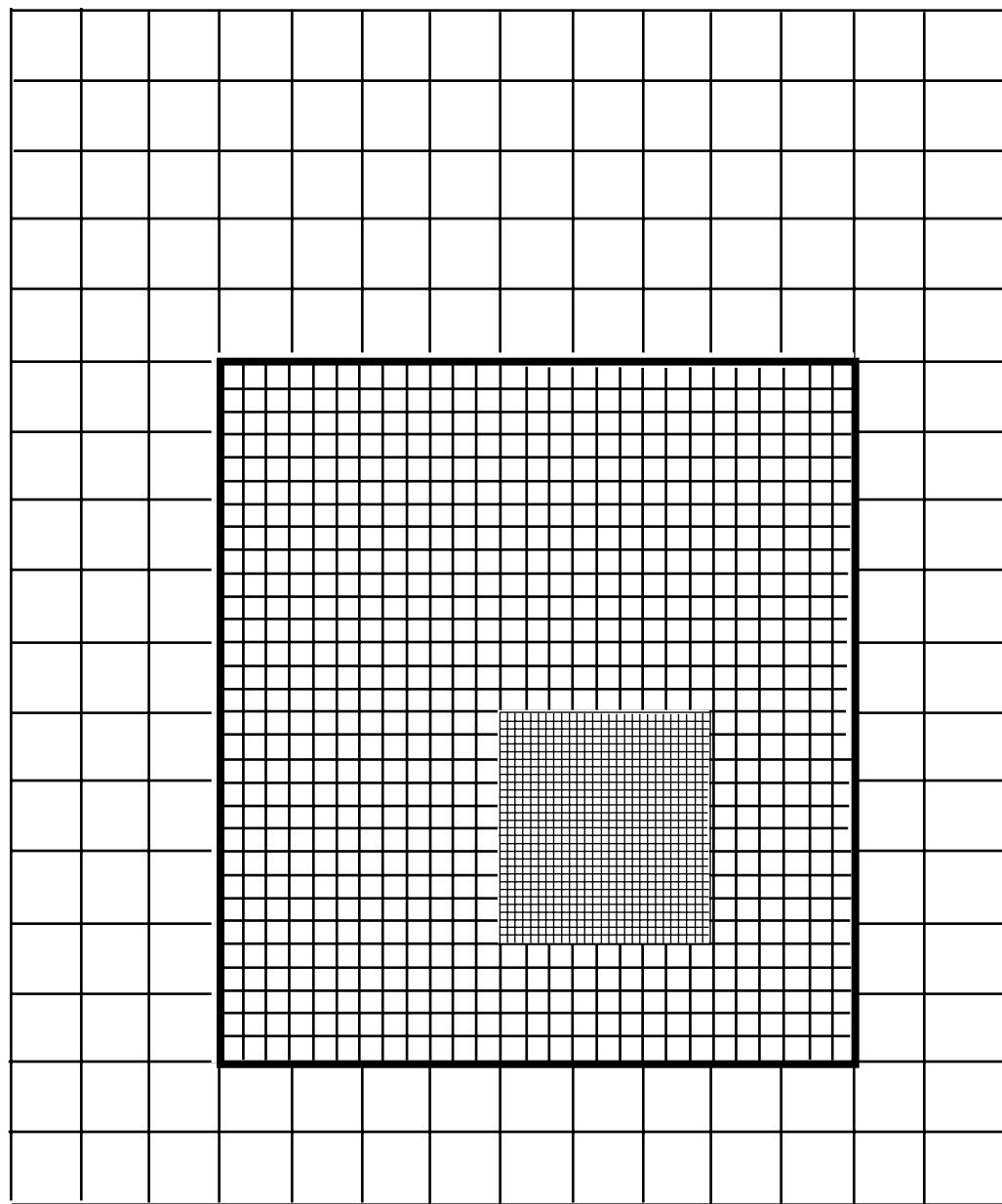
$$\frac{D}{Dt} \left(\frac{q^2}{2} \right) = \frac{\partial}{\partial x} \left[K_x \frac{\partial}{\partial x} \left(\frac{q^2}{2} \right) \right] + \frac{\partial}{\partial y} \left[K_y \frac{\partial}{\partial y} \left(\frac{q^2}{2} \right) \right] + \left(\frac{\bar{H}}{H - z_g} \right)^2 \frac{\partial}{\partial z^*} \left[q l S_q \frac{\partial}{\partial z^*} \left(\frac{q^2}{2} \right) \right]$$

$$- \frac{\bar{H}}{H - z_g} \left(\bar{u}'\bar{w}' \frac{\partial \bar{U}}{\partial z^*} + \bar{v}'\bar{w}' \frac{\partial \bar{V}}{\partial z^*} \right) + \beta g \bar{w}'\bar{\theta}'_v - \frac{q^3}{B_1 l}$$

turbulent production buoyant production dissipation

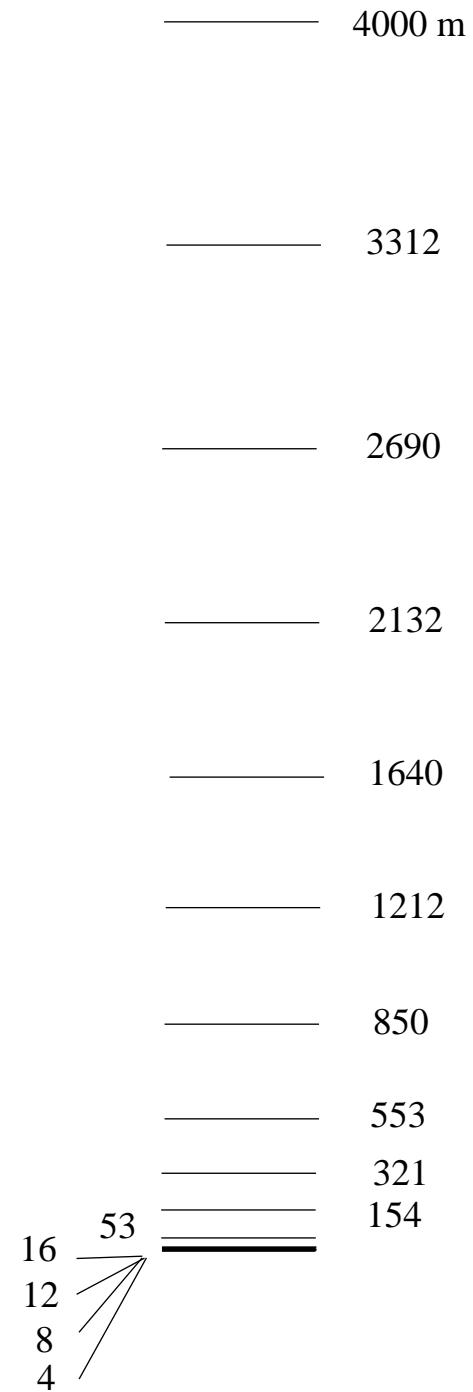
$$\begin{aligned} \frac{D}{Dt} (q^2 l) = & \frac{\partial}{\partial x} \left[K_x \frac{\partial}{\partial x} (q^2 l) \right] + \frac{\partial}{\partial y} \left[K_y \frac{\partial}{\partial y} (q^2 l) \right] + \left(\frac{\bar{H}}{H - z_g} \right)^2 \frac{\partial}{\partial z^*} \left[q l S_l \frac{\partial}{\partial z^*} (q^2 l) \right] \\ & + l F_1 \left[\frac{\bar{H}}{H - z_g} \left(-\bar{u}'\bar{w}' \frac{\partial \bar{U}}{\partial z^*} - \bar{v}'\bar{w}' \frac{\partial \bar{V}}{\partial z^*} \right) + \beta g \bar{w}'\bar{\theta}'_v \right] - \frac{q^3}{B_1} \left[1 + F_2 \left(\frac{l}{kz} \right)^2 \right] \end{aligned}$$

Nested horizontal mesh - top view



$\Delta x = \Delta y = 18, 6, \text{ and } 2 \text{ km}$

vertical grid spacing
- side view



Alternating Direction Implicit (ADI) Finite Difference Scheme

2-d example

$$\frac{\partial \phi}{\partial t} + \bar{U} \frac{\partial \phi}{\partial x} + \bar{V} \frac{\partial \phi}{\partial y} = K_x \frac{\partial^2 \phi}{\partial x^2} + K_y \frac{\partial^2 \phi}{\partial y^2}$$

$$\frac{\phi^{*} - \phi^n}{\Delta t / 2} = -\bar{U} \frac{\Delta \phi^{*}}{\Delta x} - \bar{V} \frac{\Delta \phi^n}{\Delta y} + K_x \frac{\Delta^2 \phi^{*}}{\Delta x^2} + K_y \frac{\Delta^2 \phi^n}{\Delta y^2}$$

$$\frac{\phi^{n+1} - \phi^{*}}{\Delta t / 2} = -\bar{U} \frac{\Delta \phi^{*}}{\Delta x} - \bar{V} \frac{\Delta \phi^{n+1}}{\Delta y} + K_x \frac{\Delta^2 \phi^{*}}{\Delta x^2} + K_y \frac{\Delta^2 \phi^{n+1}}{\Delta y^2}$$

where $\phi = (\bar{U}, \bar{V}, \bar{\Theta}_l, \bar{Q}_w, q^2, q^2 l)$

Alternating Direction Implicit (ADI) Finite Difference Scheme

$$\frac{\phi^* - \phi^n}{\Delta t} = \frac{1}{2}\Delta_z(\phi^* + \phi^n) + \Delta_x\phi^n + \Delta_y\phi^n - A\phi^* + F$$

$$\frac{\phi^{**} - \phi^n}{\Delta t} = \frac{1}{2}\Delta_z(\phi^* + \phi^n) + \frac{1}{2}\Delta_x(\phi^{**} + \phi^n) + \Delta_y\phi^n - A\phi^* + F$$

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{1}{2}\Delta_z(\phi^* + \phi^n) + \frac{1}{2}\Delta_x(\phi^{**} + \phi^n) + \frac{1}{2}\Delta_y(\phi^{n+1} + \phi^n) - A\phi^* + F$$

$$\phi = (\bar{U}, \bar{V}, \bar{\Theta}_l, \bar{Q}_w, q^2, q^2 l)$$

Surface Temperature B.C.

soil heat conduction equation

$$\frac{\partial \bar{T}_s}{\partial t} = \frac{\partial}{\partial z_s} \left(K_s \frac{\partial \bar{T}_s}{\partial z_s} \right)$$

heat energy balance at surface

$$R_s + R_L \downarrow - R_L \uparrow = H_s + LE + G_s$$

$$R_L \uparrow = \varepsilon \sigma T_G^4 + (1 - \varepsilon) R_L \downarrow$$

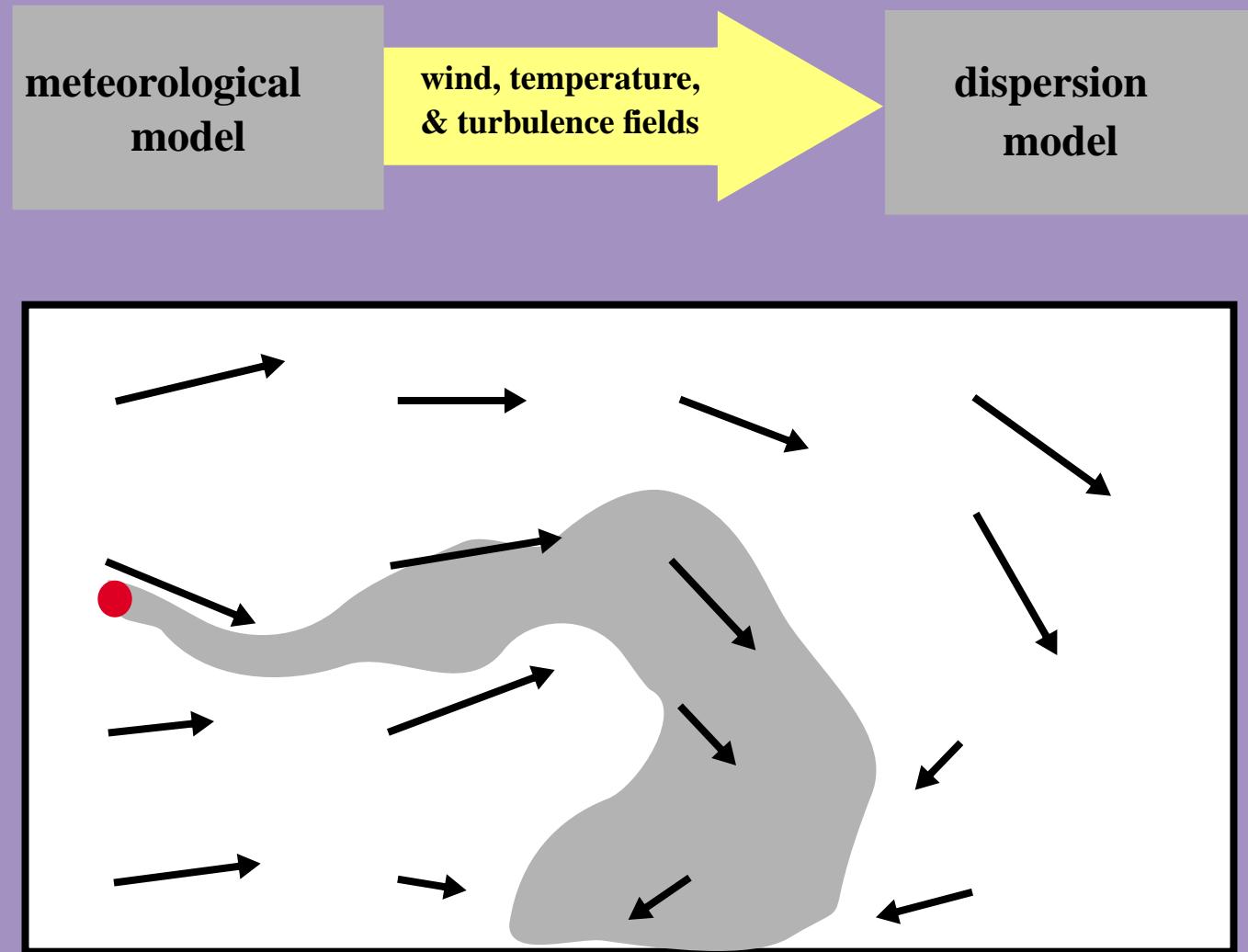
$$H_s = \rho c_p \overline{w' \theta' v} \approx -\rho_a c_p u_* T_*$$

$$B = H_s / LE$$

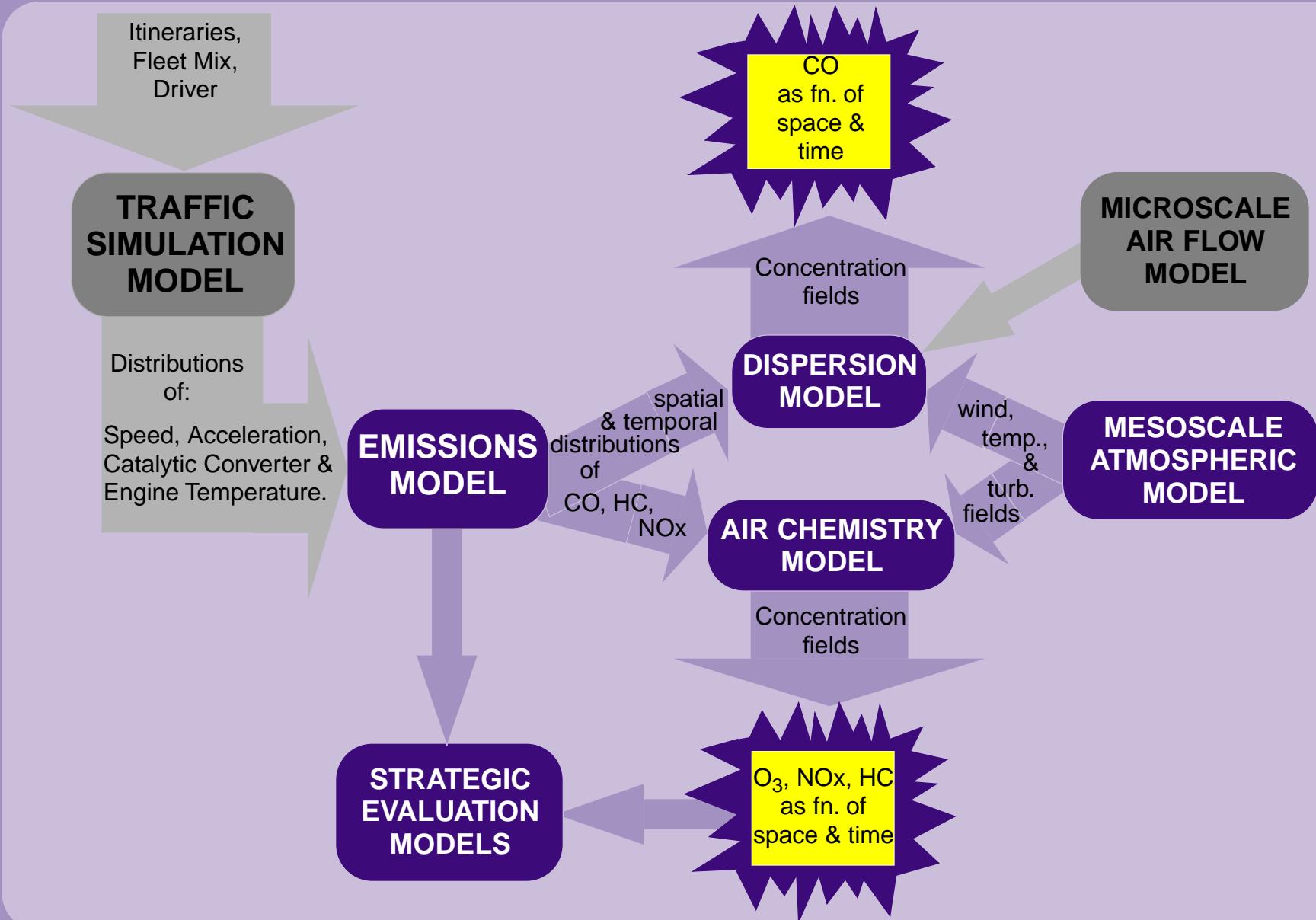
$$G_s = K_s \frac{\partial \bar{T}_s}{\partial z_s} \Big|_G$$

$$R_s + \left[\varepsilon R_L \downarrow - \varepsilon \sigma T_G^4 \right] = -\rho_a c_p u_* T_* (1 + B^{-1}) - K_s \frac{\partial \bar{T}_s}{\partial z_s} \Big|_G$$

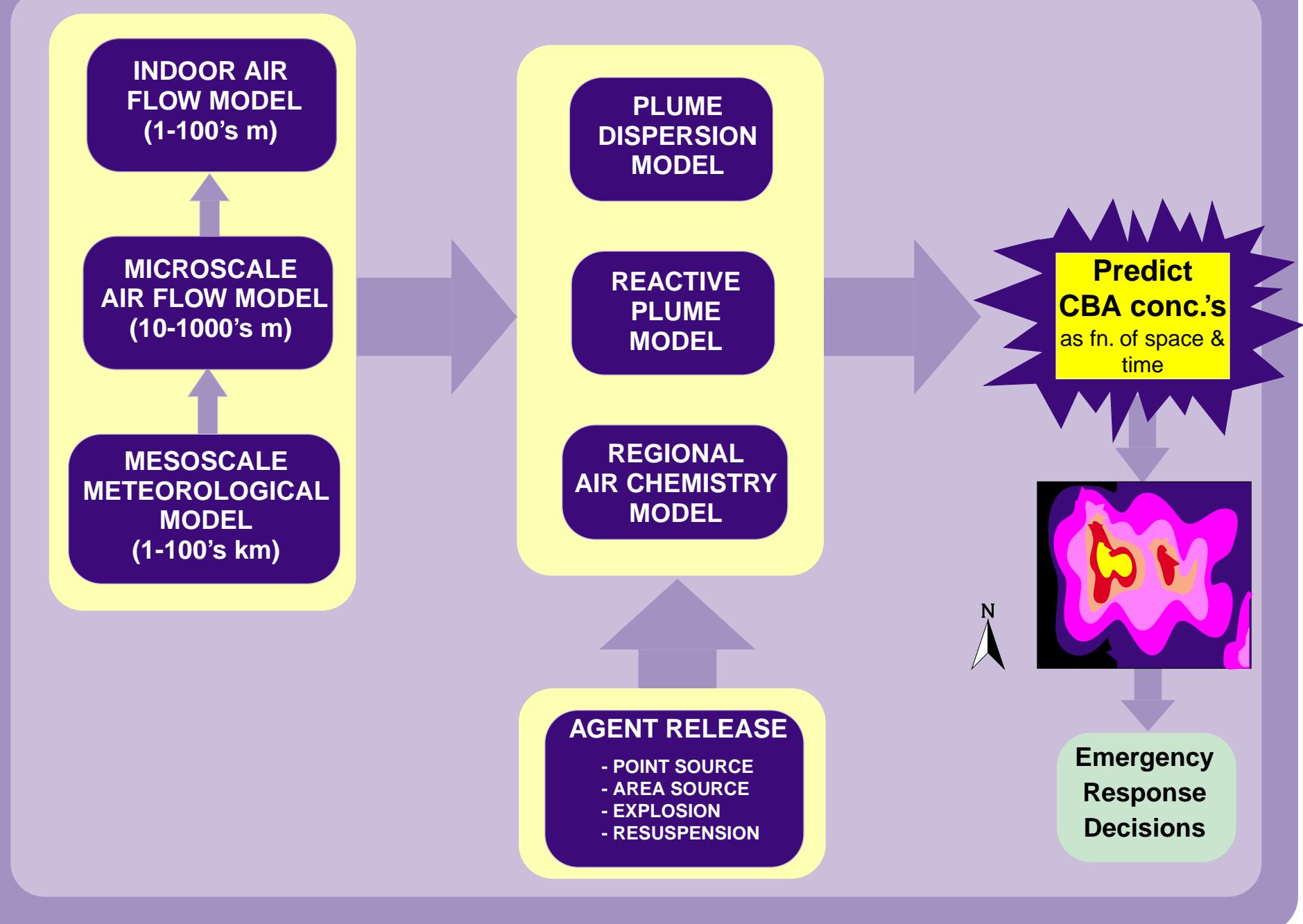
The meteorological model output is input to the dispersion model

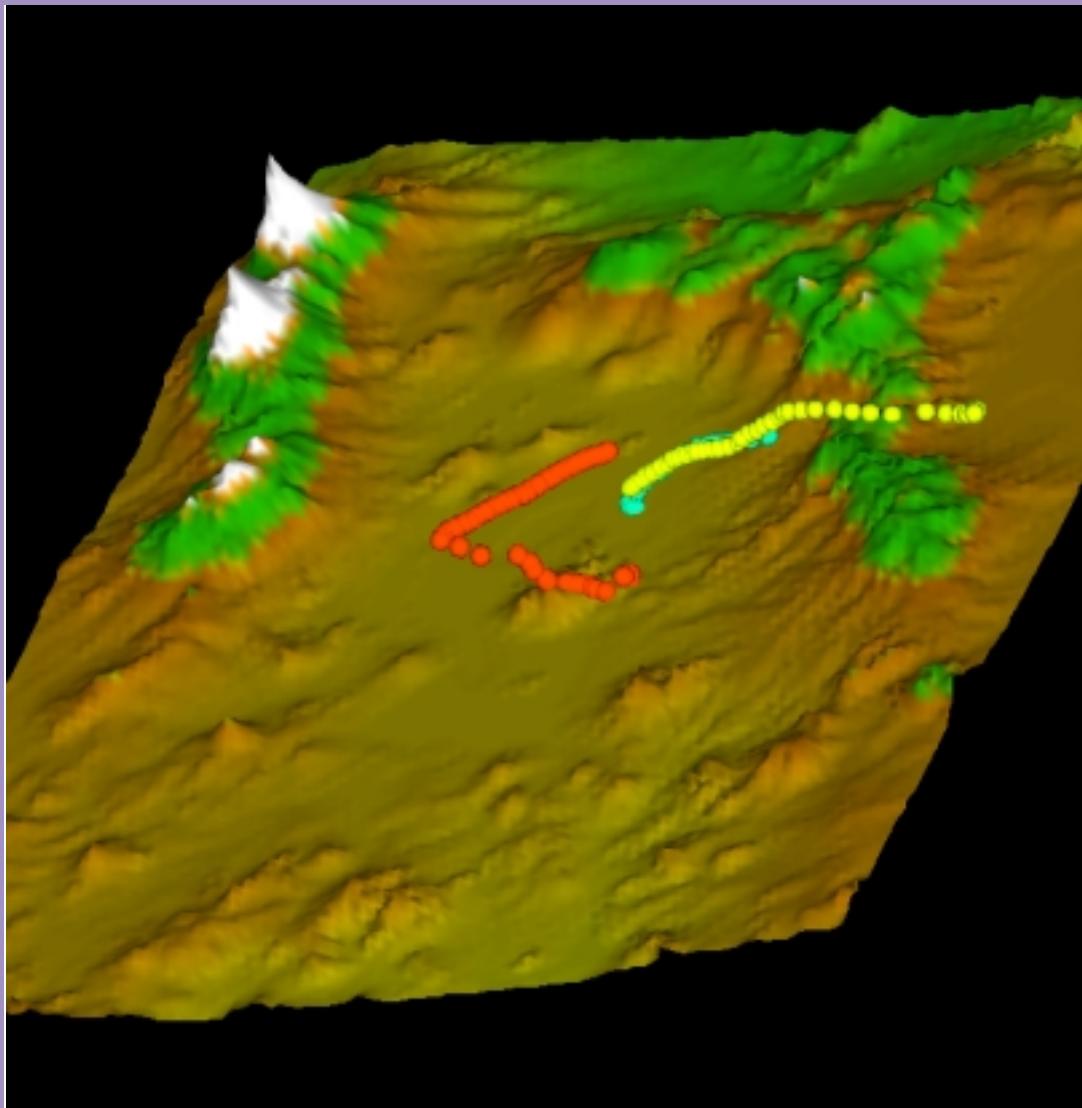


Air Pollution Modeling System



Chem-Bio Agents Transport and Fate Modeling System





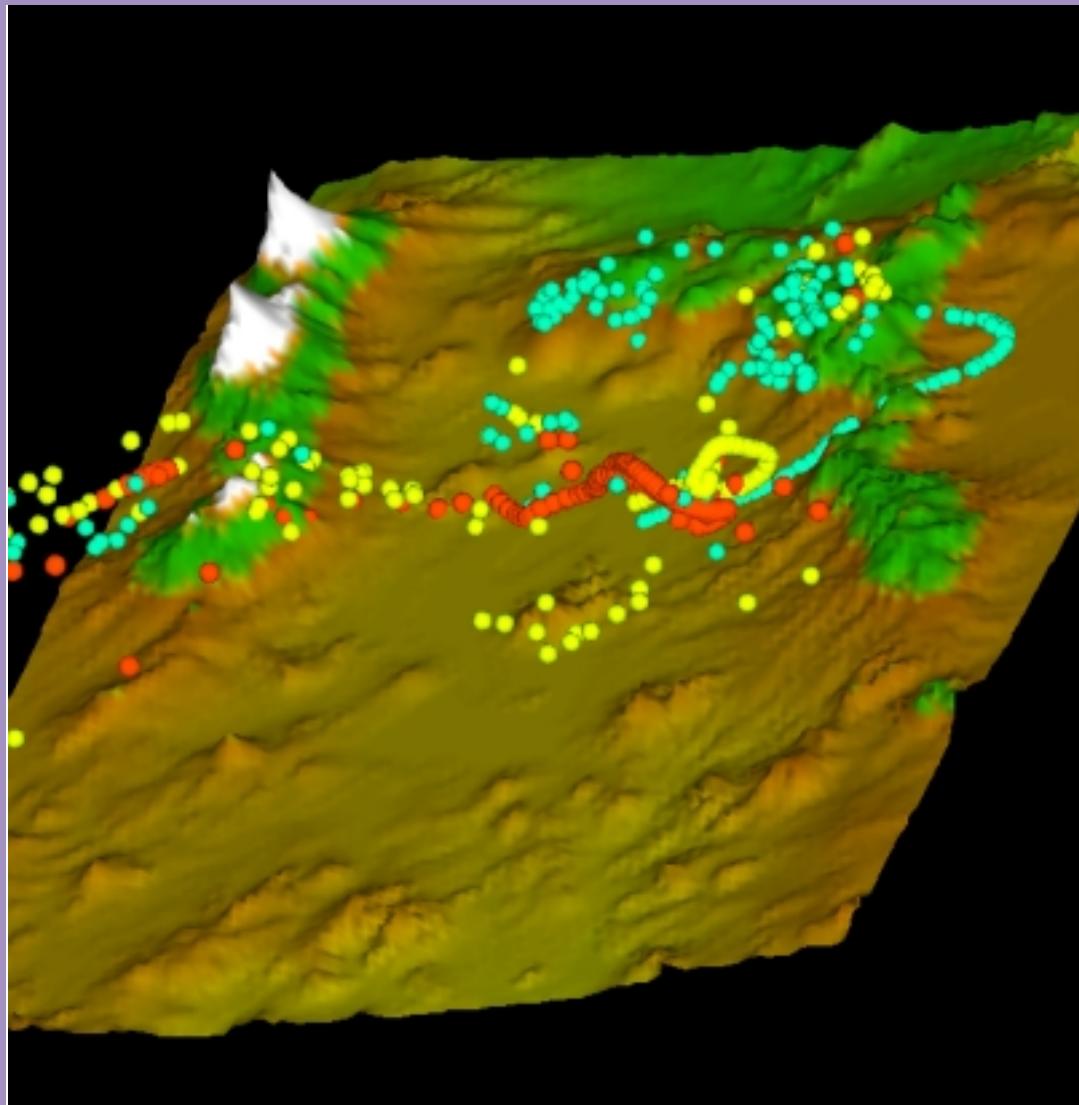
3-d time-dependent tracer simulations

Tracers released at three heights in the Valley of Mexico City using HOTMAC-produced wind fields.

The tracer simulation reveals significant vertical wind shear between the surface winds and winds aloft.

release heights:

- 20 m
- 50 m
- 1500 m



6 pm, 18 hours after release

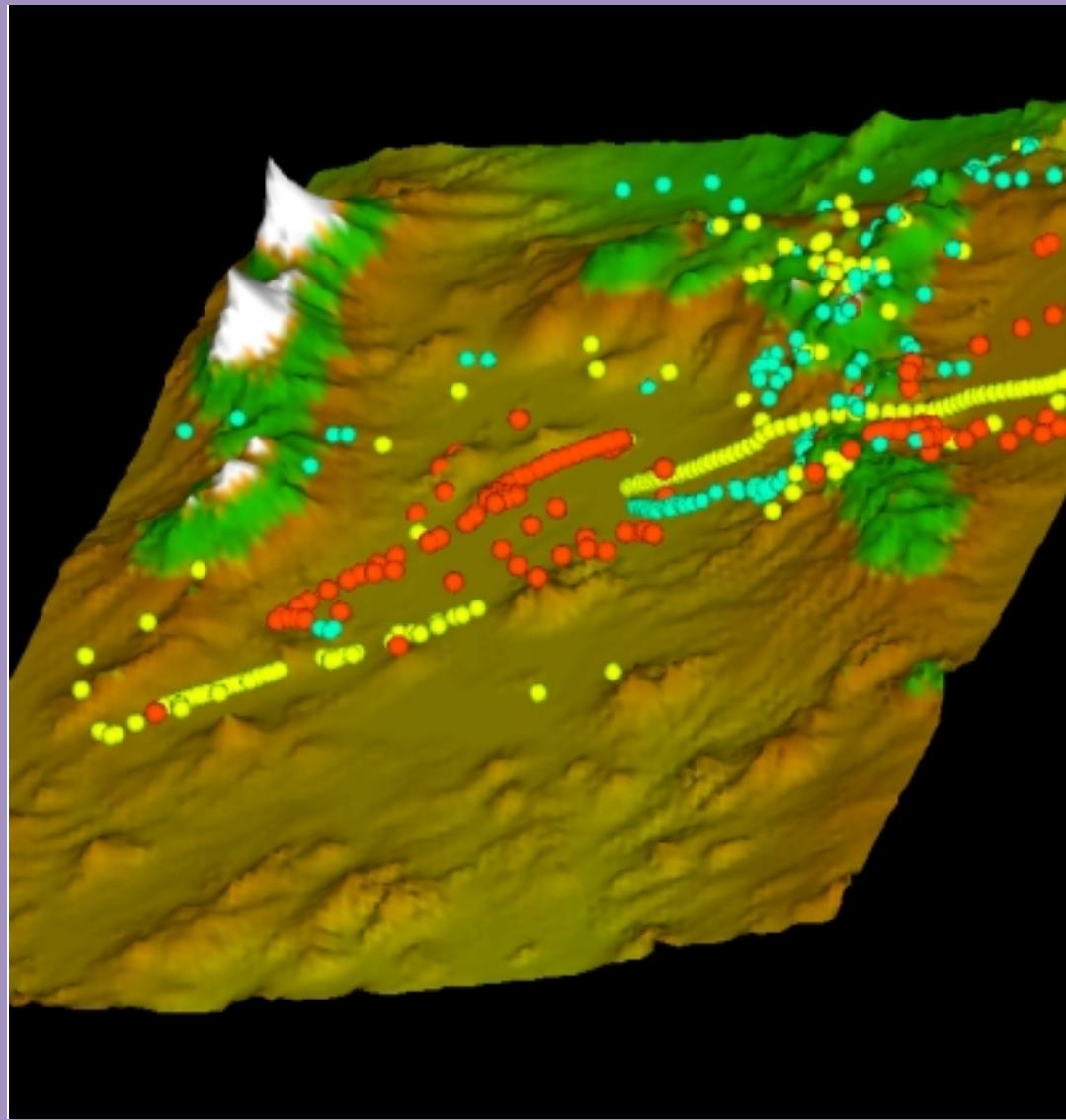
3-d time-dependent tracer simulations

Tracers released in the Valley of Mexico City using HOTMAC-produced wind fields.

The tracer simulation reveals wind shear and mountain-induced upslope and recirculation flows.

release heights:

- 20 m
- 50 m
- 1500 m



midnight, 24 hours after release

3-d time-dependent tracer simulations

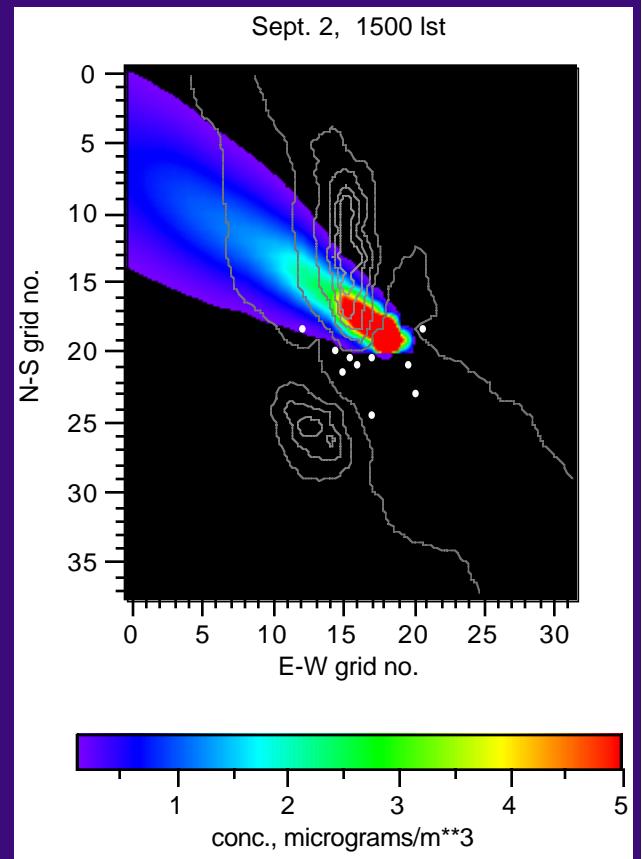
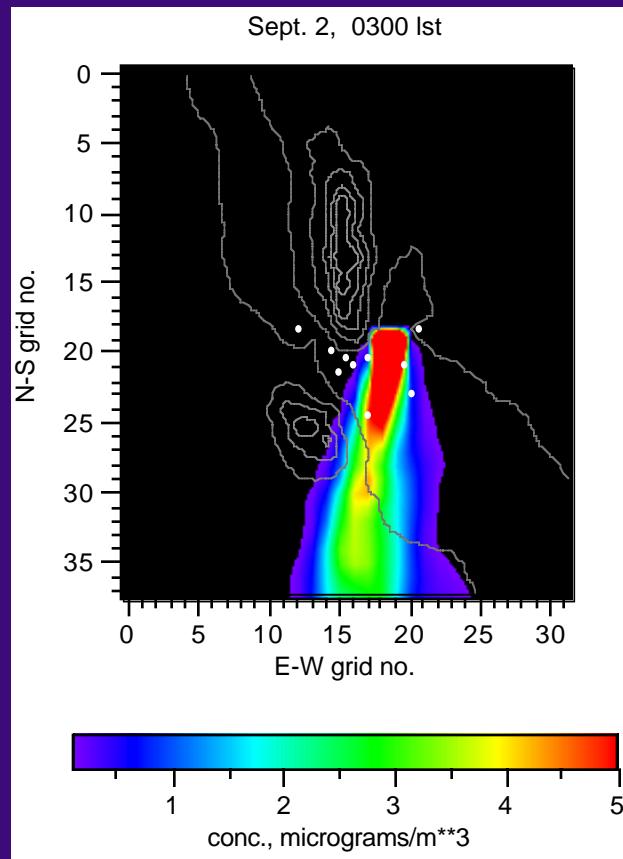
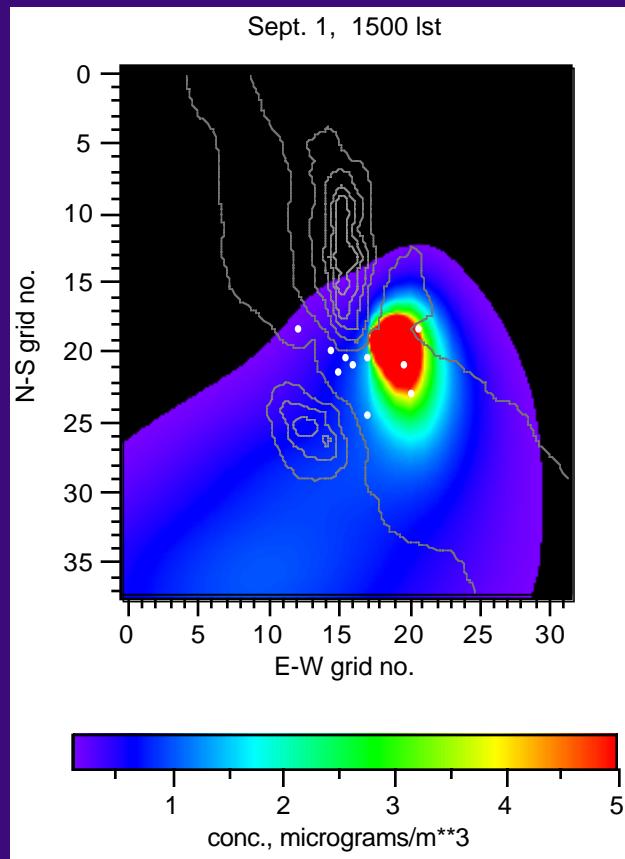
Tracers released in the Valley of Mexico City using HOTMAC-produced wind fields.

The tracer simulation reveals significant vertical wind shear and mountain-induced downslope flows.

release heights:

- 20 m
- 50 m
- 1500 m

Plume Dispersion Modeling in an Urban-Mountainous Setting

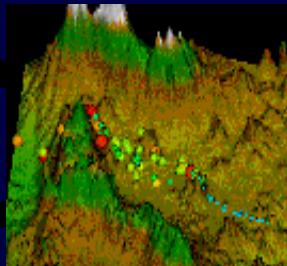


Plume dispersion simulation of a 2 km x 2 km ground source located in the El Paso/Ciudad Juarez region. Hourly-averaged surface concentration contours are shown at 12 hour intervals. The meteorological and concentration fields were computed by LANL's HOTMAC-RAPTAD modeling system. Plume concentrations change due to varying wind, temperature, and turbulence fields.

LANL: Modeling of Atmospheric Phenomena

- * **Chemical Downwind Hazard Modeling Study (Tooele Army Depot)**
- * **Mexico City Air Quality Research Initiative (MARI)**
- * **Los Alamos Emergency Preparedness Studies**
- * **Transportation Simulation Project (TRANSIMS)**
- * Chile Air Quality Program
- * ASCOT Program (Brush Creek, California Geysers, Oak Ridge, Rocky Flats)
- * Cross-Appalachian Transport Experiment (CAPTEX)
- * Lake Powell/Glen Canyon Air Quality Study
- * El Paso/Ciudad Juarez Border Air Quality Study
- * Iron Mountain Experiment and Modeling Studies

LANL Air Quality Projects



Mexico City

- meteorology
- air chemistry
- emissions
- cost-benefit analysis



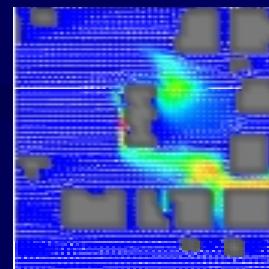
Santiago, Chile

- meteorology
- plume dispersion



Los Angeles, CA

- meteorology
- air chemistry
- stormwater transport



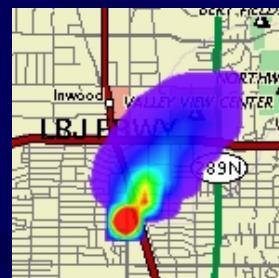
Washington DC

- flow around buildings
- plume dispersion



El Paso/Ciudad Juarez

- meteorology
- plume dispersion



Dallas, TX

- flow around buildings
- meteorology
- plume dispersion
- vehicle exposures

Applications

△ Air Pollution and Smog in Cities

- health concerns
- reduction strategies
- visibility issues

△ Air Pollution (Plume) Transport from Factories and Powerplants

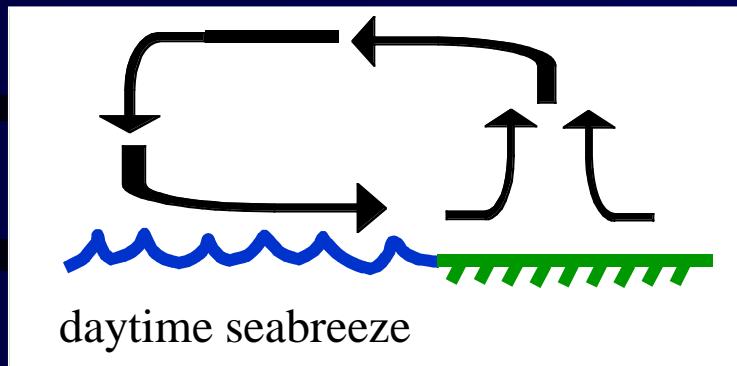
- health concerns
- reduction strategies
- visibility issues

△ Accidental Releases from Industrial, Nuclear, and Military Facilities

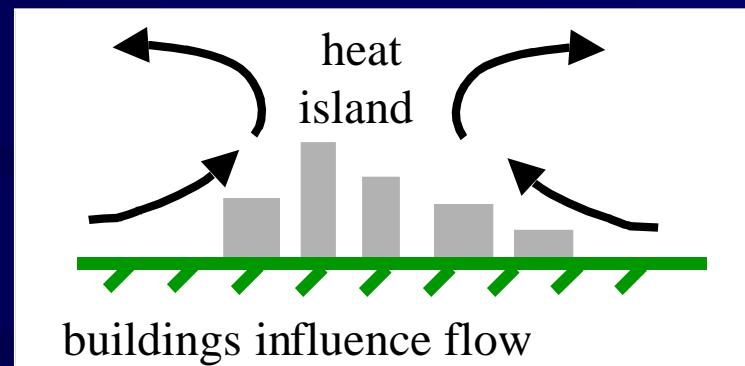
- emergency response
- planning and preparation

Special Meteorological Considerations

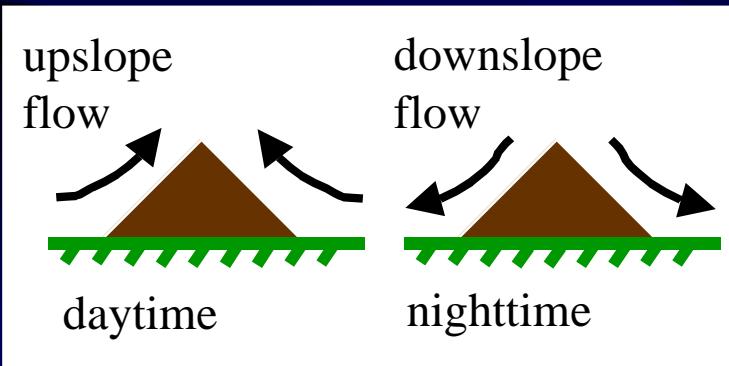
△ coastal city



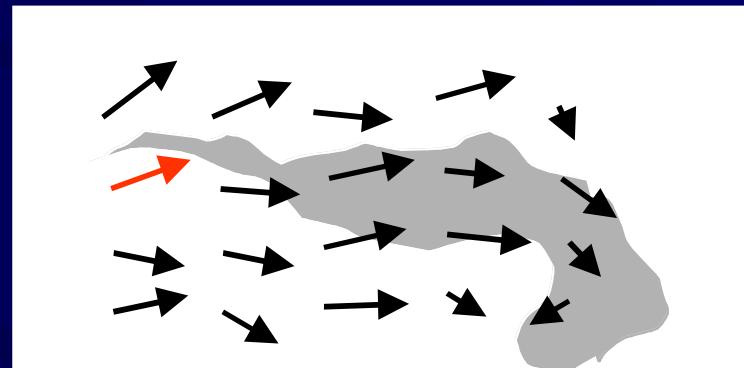
△ urban



△ mountainous terrain



△ lack of met. data



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